DAMAGE THERMODYNAMICS OF QUASIBRITTLE MATERIALS

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ABSTRACT. The description of the early stage of microfracture growth in a quasibrittle solid with thermodynamic positions is considered. From the most general thermodynamic performances the "principle" of minimization of free energy is received. The account high (down to thirds) degrees in expansion of free energy concerning parameters of a mechanical field and average microcrack energy has allowed to write down the state equation for solids with microcracks, to find equilibrium and nonequilibrium values of their average energy. From positions of a developed formalism the reason of high stability of work developments on small depths and mechanism of loss of their stability on the large depths is explained. From the fact of presence of qualitatively various behaviour of a material on the large depths the additional estimated connection between parameters of the theory is established.

Introduction

Fracture phenomena are most complicated and intrigued fundamental problem of the present-day. As of now, a sequence of fresh approaches to attacking of this problem is outlined. Statistical mechanics of cracks is most rigorous and sequential from them [7, 19], but very hard at a times. It is used out and developed the methods of the complex systems, methods of the percolation and fractal theories and setera [13]. Next way for consideration of the problem is using of purely mechanic descriptions [4, 17] and non-equilibrium thermodynamics [6, 22]. Very interest and promising results are obtained with the phase-field model [1, 8, 10, 20, 26] based on the phase transition concept [12]. In the phase-field models a order parameter describes microscopic distribution of mass density in he transition zone between a solid (phase I) and a separate crack (phase II).

It is known approaches for describing of the fracture problem as the first-order phase transition [23, 24]. One may regard an each separate crack as nucleus or droplet of new phase with determinate activation energy. Such approaches are more suitable for description of ideal zero-defects solid, for which the activation has thermal character and activation energy haven enough high value is fixed.

In the other side it is known opposite approaches for the same seemingly problem with position of the second-order phase transition [16]. Real structural inhomogeneous solids have the multitude manifest and latent defects in its bulk. They may be activated at different energies from zero for manifest defects to theoretical limit for ideal solid. Thus one may suppose that quantity of defects in a solid rests

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constant at all times, and to describe degree its activation by average energy per one defect [15, 22]. Such "order parameter" describes mesoscopic level state, a elementary unit of which consist multitude structural inhomogeneities.

Practically relaxation of quasibrittle solid with the plastic (viscous) mechanism even at slow deformation is too hard owing to large rigidity of their molecular organisation. Therefore, probably, the unique mechanism of relaxation in this case is activation and growth of microcracks, their further merge and branching (damage) and, at the end, failure thereof. The destruction of quasibrittle solid with this mechanism enough frequently is naturally observed, for example at deformation of rock around of a underground working on too large depth [2, 18, 21].

In present paper the behaviour of quasibrittle solids at high loading (deformation) is considered from general thermodynamic positions. The applicability of performances of equilibrium thermodynamics in this case is limited to intermediate temporary scale smaller necessary for diffusion healing of microcracks. From consideration are excluded both infinite timeout, and may be processes of microcrack origin. It is considered, that a real fragile solid already has natural loosenings, defects etc., which are only made active by an applied external mechanical field.

It is known the destruction is irreversible thermodynamic process. In classical thermodynamics irreversibility and non-equilibribility are taken as interrelation notes [5]. That is any irreversible process is non-equilibrium, and conversely any non-equilibrium one is irreversible. It is true for infinite slow processes. In real situation of intermediate time there is possibility when process has irreversible character, but one is equilibrated or more precisely quasiequilibrated.

1. Constitutive relations

The occurrence of microcracks (damage) conducts to growth of internal energy of a solid on value of work of external force equal to total energy of the broken off bandings. In this case for slow equilibrium processes basic equation of thermodynamics is possible to write down as:

(1)
$$du = Tds + \sigma_{ij}d\varepsilon_{ij} + \varphi d\nu,$$

where u - is density of internal energy, J/m^3 , T - is temperature; s - is density of entropy, $J/degree*m^3$, σ_{ij} - is tensor of stress, N/m^2 ; ε_{ij} - is reversible (elastic) part of deformation tensor; φ , ν - is accordingly average additional energy of system per one microcrack, J, and thermodynamically paired quantity, connected to it having dimension of microcrack density, m^{-3} . The relationship (1) can be presented in other, more known form

(2)
$$du = Tds + \sigma_{ij}d\varepsilon_{ij} + \sigma_{ij}d\varepsilon_{ij}^{n},$$

where ε_{ij}^n - tensor of inelastic deformations. From the given expression it is visible, that "pumping" of internal energy is carried out through an irreversible part of work of a external stress. As other channels of dissipation are not considered, this part of work can go on "pumping" of internal energy in the form or thermal movement (that is taken into account by first term in (1)), or in the form surface energy and energy of microcracks interaction (that is taken into account by last term in (1)). The form of the relationship (1) is more convenient, if the research of a model of a solid are limited to energetic level of consideration, that, however, it is

quite enough for reception of many useful and common results. If necessary of more detailed analysis between macroscopic parameters σ_{ij} , ε_{ij}^n and internal ones φ , h is necessary to establish additional connection similar those in the thermodynamic theory of dislocations [11].

In essence, the relation (1) is tantamount to stating that irreversible part of external work is substituted with effective external microcrack flow in a manner like thermal flow. Motivation for such presentation is concluded that information about solid state in form of inelastic deformation is lost for system. In other side this information residues in the system in the form it's changed microcrack structure. In this context there is quite deep analogy between first and last terms of expression (1). Namely, temperature T has meaning of average energy per one particle rather per one degree of freedom, while entropy has meaning of measure of such effective degree of freedom. Parameter φ , as reported above, has meaning of average additional energy per one defect (in our case, microcrack), that is it plays a role of static "temperature". Logically to surmise that density of microcracks is some analogue of static "entropy". Really, when system transits from a nonequilibrium state to it's equilibrium one both entropy and density of microcracks have similar feature: namely at suit external conditions each of them tends to increasing. It is necessary to note, that the additional internal energy connected to occurrence of a separate microcrack, is proportional to the sizes by last, and the increase of average energy of microcracks is equivalent to increase of their average size. This additional energy is caused by direct break of banding, formation of a free surface limiting a microcrack, and reorganization of nuclear layers near the surface with arising of additional internal stress.

Free energy of a system is such part of it's internal energy, which is able to perform mechanical work. Unavailable energy is that lost part of internal energy, which isn't able to perform mechanical work. The thermal part of unavailable energy is well known and equal to Ts. It is clear, that part energy accumulated in the microcracks is lost for work too. In the context of said above let this part of unavailable energy be equal to $\varphi\nu$. Then new expression for density of free energy first has been wrote in the form:

$$f = u - Ts - \varphi \nu,$$

so, that its complete differential can be written down in the form

$$df = -sdT + \sigma_{ij}d\varepsilon_{ij} - \nu d\varphi,$$

Ignoring by thermal contribution one may rewrite down (4) as

$$df = \sigma_{ij} d\varepsilon_{ij} - \nu d\varphi,$$

From a relationship (5) follows, that the free energy is potential, if variables ε_{ij} , φ are chosen as arguments, i.e. $f = f(\varepsilon_{ij}, \varphi)$. If the explicit arguments dependence of free energy density was known, variables σ_{ij} and ν thermodynamically connected with arguments could be determined by simple differentiation:

(6)
$$\sigma_{ij} = \frac{\partial f}{\partial \varepsilon_{ij}}, \nu = -\frac{\partial f}{\partial \varphi}.$$

It is necessary to note, that on sense of the relationship (1), the relationships (6) should express external influences on elementary unit. At the same time parameter ν can make sense of external parameter only for the mobile defects capable to move through external interface of elementary unit. If the defects are motionless, and can only arise or disappear inside volume, that, strictly speaking, it is necessary to put $\nu = const$. Without the loss of generality it is believed that const = 0. Validity of some extreme "principle" from here follows [9, 12]:

(7)
$$\frac{\partial f}{\partial \varphi} = 0.$$

By this meant that in the equilibrium stationary state the irreversible work isn't carried out. If one exerts additional constant stress new microcracks are arisen (activated) in the bulk for as long as new equilibrium state is achieved. In the other side condition (7) is meant the free energy has minimum in any equilibrium state as φ is conceptually internal parameter.

2. Expanding at power series

As the definition of an explicit expression for free energy density is a hard task, we apply standard in such cases reception, namely, we shall expand free energy on its arguments:

(8)
$$f(\varepsilon_{ij},\varphi) = f_0 - \nu_0 \varphi + \frac{1}{2} a \varphi^2 - \frac{1}{3} b \varphi^3 + \frac{1}{2} \lambda \varepsilon_{ii}^2 + \mu \varepsilon_{ij}^2 - g \varphi \varepsilon_{ii} + \frac{1}{2} \overline{\lambda} \varphi \varepsilon_{ii}^2 + \overline{\mu} \varphi \varepsilon_{ij}^2 + e \varphi^2 \varepsilon_{ii} + \dots$$

First term f_0 is free energy of the non-loaded body in absence of microcracks. The following three terms describe features of dependence of free energy from microcracs in absence external mechanical load. Term $\nu_0\varphi$ is meaningful to bulk density of superficial energy of the completely isolated and not interacted among themselves microcracks (ν_0 - is their natural density). Square term with φ describes dimensional effect taking into account that fact, that the growth of energy of a microcrack with increase of its size is slowed down. Cubic term with φ takes into account an opportunity of merge of microcracks, when the average energy per one merged microcrack, grows at common reduction of energy of system (sign "minus" at b > 0).

Terms $\lambda \varepsilon_{ii}^2/2$ and $\mu \varepsilon_{ij}^2$ in (8) describe decomposition of an elastic part of energy through invariant of deformation tensor in a continuous solid (in absence of microcracks).

Subsequent mixed terms have double interpretation: from the point of view of influence of microcracks on deformation field and, on the contrary, from the point of view of influence of deformation field on behaviour of microcracks. Term $-g\varphi\varepsilon_{ii}$, on the one hand, takes into account loosening up (increase of volume) non-loaded material at presence of microcracks, and, on the other hand, change of "own" energy of microcracks owing to work of mechanical forces.

Cubic mixed terms $\overline{\lambda}\varphi\varepsilon_{ii}^2/2$ and $\overline{\mu}\varphi\varepsilon_{ij}^2$ also describe increase or reduction of free energy at the expense of the uncoordinated deformation of various elementary volumes, for which size of average energy of microcracks φ (or their average size) is a measure of such incoordination. As a matter of fact, these terms describe additional interaction of elementary volumes, however only formally they can be

treated as effective interaction of microcracks. The given interaction is carried out through far-acted field of macroscopic deformations. It is need to distinguish such interaction from interactions of own deformation field of microcracs, which decreases quickly enough [3] and can play an appreciable role only at large density of microcracks. The parameters $\overline{\lambda}, \overline{\mu}$ in this context take into account change of stiffness of a material for the account of microcracs. Discussed terms are possible to interpret and as influence on energy of a microcrack of deformation field owing to the same uncoordinated deformation.

At last, term $e\varphi^2\varepsilon_{ii}$ describes, on the one hand, smaller growth of a degree of material loosening with growth of the microcrack sizes, with another - influence of interaction through own deformed field. Notice that the centre of the expansion may be not only zero as in (8), but any other value of φ .

Leaving in (8) explicit dependence only from average energy of microcracks, we receive:

(9)
$$f(\varphi) = \overline{f_0} - \overline{\nu}\varphi + \frac{1}{2}\overline{a}\varphi^2 - \frac{1}{3}b\varphi^3 + ...,$$

where

(10)
$$\overline{f_0} = f_0 + \frac{1}{2}\lambda\varepsilon_{ii}^2 + \mu\varepsilon_{ij}^2$$

$$\overline{\nu} = \nu_0 + g\varepsilon_{ii} - \frac{1}{2}\overline{\lambda}\varepsilon_{ii}^2 - \overline{\mu}\varepsilon_{ij}^2$$

$$\overline{a} = a + 2e\varepsilon_{ii}.$$

The diagram of free energy generally represents a cubic parabola, the variants of possible forms of which and arrangement of them concerning of coordinate axes at various values of tensor components of deformation are given in the fig. 1. Three forms of a cubic parabola - with two extremes on the diagram, with a point inflexion and monotonously falling down diagram (fig. 1a) are generally possible. From extreme "principle" (7) the equation for definition of equilibrium values of average energy follows

(11)
$$f'(\varphi) = -\overline{\nu} + \overline{a}\varphi - b\varphi^2 = 0.$$

The decisions of the equation

(12)
$$\varphi_{1/2} = \frac{1}{2b} (\overline{a} \pm (\overline{a}^2 - 4b\overline{\nu})^{1/2})$$

are those, that is valid $\varphi_1 > \varphi_2$. The stability of roots of the equation (11) is determined by sign of the second derivative of free energy:

(13)
$$f''(\varphi_{1/2}) = \overline{a} - 2b\varphi_{1/2} = \mp (\overline{a}^2 - 4b\overline{\nu})^{1/2}),$$

The first root is unstable, second one is steady and determines some equilibrium value of average energy come on one microcrack. As the state of a solid with microcracks, strictly speaking, is nonequilibrium, but can exist long enough, it as a matter of fact is metastable. The extreme principle in the form (11) determines conditions of existence of its metastable state. If the deviation of the current value of average energy from equilibrium is insignificant, the solid keeps the integrity .

Here it is meant, that the current value of average energy of microcracks can, both lag behind, and outstrip equilibrium value, which with (12) follows change of a mode of elastic loading of a sample. If the current value of average current average energy is those, that, the system passes on a falling down branch of free energy (curve 1, fig. 1a), that is equivalent to creep or later to macroscopic destruction of a solid or, at least, to transition of destruction to the following structural level (merge of microcracks). Existence of a potential barrier separating a steady state from of the falling down branch, depends from sign of the discriminate:

$$(14) D = \overline{a}^2 - 4b\overline{\nu}.$$

At D=0 (curve 2, fig. 1a) the potential barrier is absent. In this case body begins to creep at slightest change of parameter φ . At negative values of discriminant (curve 3, fig. 1a) the equilibrium values are absent at all, and the solid creeps constantly. Under condition D>0 it takes place two different decisions, between which should be observed an inequality $\varphi_1>\varphi_2$. Increasing deformation of a material so that to pass from negative values of discriminant D to positive them, it is possible to transfer a solid from a conditionally equilibrium state to nonequilibrium state. In result the value of average energy of microcracks will grow continuously (creep), that will be achieved for the account, both growth of the sizes of separate microcracks, and their merge at general downturn of energy of system. Value D=0 separates regions of equilibrium states and creep. Further, varying the free energy on deformation, it is possible to determine a field of pressure:

(15)
$$\sigma_{ij} = \frac{\partial f}{\partial \varepsilon_{ij}} = [(\lambda_{ef} \varepsilon_{ii} - g\varphi)\delta_{ij} - 2\mu_{ef} \varepsilon_{ij}],$$

Where

(16)
$$\lambda_{ef} = \lambda + \overline{\lambda},$$

$$\mu_{ef} = \mu + \overline{\mu}$$

As it is visible, the elastic modules is varied of depending on presence of microcracks. The positive values of parameters $\overline{\lambda}$ and $\overline{\mu}$ ($\overline{\lambda}>0$ and $\overline{\mu}>0$) correspond to growth of effective stiffness of a material with growth of average microcrack energy. The last takes place, if during deformation, despite of break of a part of the bindings the rest of them are capable to keep additional action promoting more hard response. Growing of average microcrack energy may be accompanied by strengthening of rest bonds with increasing of internal stress around a microcrack. If it not so, the break of bindings will cause downturn of rigidity of a material, and the inequalities $\overline{\lambda}<0$ and $\overline{\mu}<0$ will be carried out. The first case is quite exotic, but the letter one is thermodynamically more correct.

3. Transition through zero

As to metastable states correspondingly dependence of sign of the parameter φ_2 three qualitatively various situations are possible. The positive values of this parameter (curve 3, fig. 1a) describe a real physical state of a solid. The negative values (curve 1, fig. 1a) have no physical sense, and the free energy formally does not depend in any way on microcracks. The independence of free energy of parameter

 φ in the field of its negative values is represented by horizontal lines (fig. 1a). The equality to zero of this parameter determines the instant of disappearance (in statistical sense) microcracks for the reason that their sizes at zero their average energy are equal to zero (collapse).

We shall consider features of transition of system through zero of equilibrium parameter φ_2 . Near to this point the large powers in expansion of free energy it is possible to reject and to be limited only to square-law approximation. Then the point $\varphi_2 = 0$ is achieved at deformation with hydrostatic compression:

$$\varepsilon_{ii}^{(0)} = -\frac{\nu}{q} < 0,$$

To the left of a point $\varphi=0$ the free energy, as was told above, does not depend from variable φ and, hence, it's derivative of all orders on this variable identically address in zero. To the right of a point $\varphi=0$ derivative from free energy are not equal to zero and can be determined by double differentiation of expression (8). Thus, second derivative of free energy will have discontinuity at transition of a point $\varphi=0$:

(18)
$$f_{\varphi}'' = \overline{a} = 0...if....\varepsilon_{ii} > -\frac{\nu}{g} < 0,$$
$$f_{\varphi}'' = 0....if....\varepsilon_{ii} < -\frac{\nu}{g} < 0,$$

And also

(19)
$$f_{\varphi,\varepsilon_{ii}}'' = -g > 0...if....\varepsilon_{ii} > -\frac{\nu}{g} < 0,$$
$$f_{\varphi,\varepsilon_{ii}}'' = 0...if....\varepsilon_{ii} < -\frac{\nu}{g} < 0,$$

In second by derivative on deformation the discontinuity is absent, but the break on the diagram of dependence from parameter φ takes place. The behaviour and character of two derivatives free energy discontinuity testifies that we have to deal with some analogue of a second kind phase transition.

4. "Elastic-creep" transition

The presented here theory can be applied to qualitative explanation of a phenomenon of destruction of rock around of underground workings. It is known, that ones carried out on small depths have enough large stability. Around workings carried out on large depths the phenomena of the abnormal large displacement of rock are observed. This is cause fast reduction of section of working and, eventually, its complete destruction [25]. According to the theory at small deformation, ε_{ii} this is at small depths (the estimates are given below) for rock around working, will be satisfied condition of existence of an equilibrium state (case D < 0), which is described by free energy with one minimum. (curve 1 in the fig. 1a). At increase of shear deformations (the bulk deformation in elastic approximation is equal to zero), this is at the large depths, the character of dependence of free energy will change, and it will be described already by curve which is not having extremes (a curve 3 on the fig. 1a). In this case system has no equilibrium states (at D > 0) and, hence, will be constant to creep.

Own to creep system evaluates in the side of growing of average microcrack energy. After a time system lands in region of a large φ and power expansion of free energy (8) becomes not true. The state becomes exclusively non-equilibrium and new assumptions are need for description of system. For example, one can assume that creep changes medium parameters with rate in proportion to deviator of stress tensor [14] and so on.

The described above phenomenon prompts a graceful way of an establishment of estimated connection between parameters of the theory. Let's assume, that depth H of a working, since which the specified phenomenon begins to be shown, is equal 200m. The hydrostatic pressure, appropriate to it, makes γH , and tangential tensor component of pressure on a contour of the working is $2\gamma H$ (where $\gamma = \rho g$, ρ - is density of rock equal on the average $2.6*10^3 kg/m^3$, g - is free fall acceleration). From here $\sigma_{\tau} = 10.4 MPa$. Believing, that shear stiffness of a rock 30GPa, for shear components of deformation tensor we receive value of the order $\varepsilon_{\tau} = \sigma_{\tau}/\mu = 0.00035$. The square of this value has the order second tensor invariant of deformations ε_{ij}^2 appearing in expanding of free energy (8). Taking into account, that on contour of the working first tensor invariant of deformation is identically equal zero (it follows from exact decision of the problem in elastic production), from condition of equality zero of a determinant (14) is possible to write down as:

(20)
$$a^2 - 4b(\nu_0 - 0.00035\overline{\mu}) = 0.$$

The given connection between parameters of the theory, alongside with attraction of results of special experiments, can be useful to numerical estimate. At the present moment the complete complex of such experiments directed on measurement of parameters $a, b, \nu_0, \overline{\mu}$, and other parameters of the theory, to my mind, are absent. The offered here consideration can serve as stimulus for development of experimental development in this direction.

5. Practical sequels

From the above an original idea of increasing of opening stable in the Mining field is followed. The much troubles with traditional ways for opening timbering is - one combats with no cause, but with effects.

Usual evolution of natural fracture of rock around opening passes through such stages as a) accumulation of microcracks and b) macroscopical fracture

The first stage has rate in proportion to value of nonequilibrium factor (intensity of stress tensor deviator) with maximum on the "free" surface on the opening. The second stage passes by means of microcrack association with production of randomly oriented internal surfaces and with rock breakage maximum on the "free" surface of the opening.

Random character of the internal surfaces orientation has led to a situation, when among multitude of rock fragments may be found such, which have acute angle directed in opposition to the "free" surface. As a consequence with relative ease they may be displaced in the region of the free space of the opening under a pressure of another fragments. The availability of such fragments sharply decreases the stability of rock toward further fracture. Fracture covers larger and larger region of rock massive, that sharply reduces net section of the opening and requires major repairs of it.

The crux of the way next one mustn't wait as long as rock massive will be collapsed as unwanted, but one may specially destroys it as necessary. It should be prevented the generation of fragments described above by means of timely cutting of fragments with such orientations of its faces, which are favored for further locking. Moreover, the removal of some part of matter in result of cutting will have led to its partly or total unloading and to transfer of maximum of support pressure (and nonequilibrium factor too) in the region of basements of cut rock fragments. The transfer of maximum of nonequilibrium factor at certain distance from "free" surface into rock massive forms conditions for accumulation of microcracks in this distance and for further macroscopical fracture along region covering the basements of cut fragments. Such fracture is favorable to finish separation of cut fragments from the main rock massive. This is tantamount to creating of a firm rock ring playing a role of power rock casing for the rest of rock massive. During fracture in the internal region both loading of the rock ring will increase and its reverse action on the fracture region will decrease nonequilibrium factor and as consequence will slow down the fracture in the whole.

Thus the "partition" of massive by the offered way will have led to essential (at favor conditions in many times) increasing of stability and lifetime of a opening. Moreover, at favor conditions (firm rock, absence of foliation, tectonic dislocations and cetera) it is possible dispense with traditional synthetic timbering and to limit with light closed support. For execution of way one must cut rock massive around a cylindrical opening on fragments with some plans. The firsts of this plans must approximately pass through the axis of the cylindrical opening, the another are approximately oriented at right angles to axis (along contour of the opening). The distance between cuttings, its depth, form and cetera are questions for principal new technology in the Mining.

6. Conclusions

Introduction in the basic ratio (1) thermodynamics of such internal parameters, as average additional energy per one microcrack, and density of microcracks, has allowed to give the physical contents, apparently, to only mechanical task of destruction of a material and to apply to its analysis standard methods.

The condition of absence of external sources of microcracks has allowed to deduce extreme property of free energy (consisting in equality to zero by its by first by derivative on internal parameter) from the general positions of thermodynamics, instead of postulate it as a separate principle.

The equilibrium values of internal parameter are found and the discontinuity of the second derivative free energy are determined at transition through zero of average energy come per microcrack. The equation of a state (18) for a body with microcracks and expression (19) for effective elastic modules is received.

The developed approach allows to describe process of destruction of solids from uniform thermodynamic positions. The feature of destruction of such solids is that under action of mechanical pressure all kinds genetic discontinuity - microcrack, micropores, easing etc., always available in any real solid are made active. At small mechanical influences there is some average size of microcracks responding an equilibrium state. Since enough large level of mechanical pressure, the equilibrium state degenerates, and the system passes in a nonequilibrium mode. In this mode

there is a unlimited growth and merge of microcracks (creep) resulting, at the end, to macroscopic destruction of a solid. See Figure 1

With the help of a developed formalism it is possible simply enough to explain the reason essential (under the order of size) distinction of stability of rock around workins on small and large depths.

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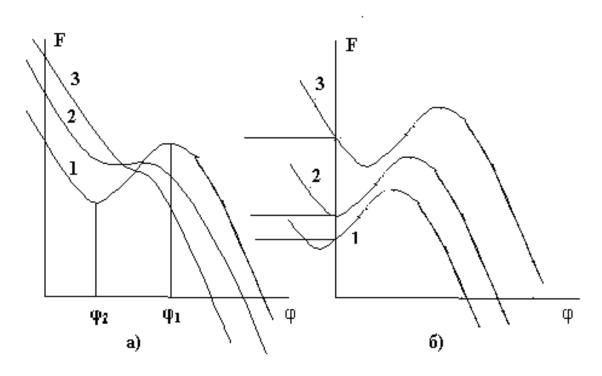


FIGURE 1. Variants of the diagrams of free energy: a) at various values of discriminant D: 1) - D ; 0; 2) - D=0; 3) - D ; 0; b) at various signs of φ_2 : 1) - φ_2 < 0; 2) - φ_2 = 0; 3) - φ_2 > 0.